

ATOMIC opacity calculations using CHEMEOS

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The new ATOMIC code

- Another Theoretical Opacity Modeling Integrated Code
- ATOMIC = FINE + LEDCOP + CHEMEO
- J. Abdallah, J. Colgan, C. Fontes, P. Hakel, D. Kilcrease, N. Magee, S. Mazevet, M. Sherrill, H. Zhang
- low-Z opacity and equation of state code
- both LTE and non-LTE conditions
- plasma effects / continuum lowering

The equation-of-state (EOS) model

- tested against quantum molecular dynamics (QMD) and path-integral Monte Carlo (PIMC) calculations for hydrogen and helium
- application to heavier elements (C, O, Ar)



LTE: free energy minimization

- chemical picture
- ensures thermodynamic consistency of the model
- yields LTE population distribution $\{ N_s \}$
- plasma and EOS characteristics can be obtained as derivatives of the free energy $F(V, T, \{ N_s \})$
 - pressure:

$$P = - \left(\frac{\partial F}{\partial V} \right)_{T, \{N_s\}}$$

- energy:

$$E = -T^2 \left(\frac{\partial(F/T)}{\partial T} \right)_{V, \{N_s\}}$$

W. Däppen, L. Anderson, and D. Mihalas: Ap.J. **319**, 195 (1987)

D. Saumon and G. Chabrier: Phys. Rev. A **44** (8), 5122 (1991); **46** (4) 2084 (1992)

G. Chabrier and A.Y. Potekhin: Phys. Rev. E **58** (4), 4941 (1998)



Occupation probability formalism

- models the elimination of bound states by dense plasma effects (e.g., microfields)
 - "gentle" truncation of partition functions (LTE)
 - modified atomic kinetics rate equations (NLTE)
- allows for a smooth merging of bound-bound and bound-free sections of the spectrum (edge lowering/broadening)

D.G. Hummer and D. Mihalas: Ap.J. **331**, 794 (1988)

D. Mihalas, W. Däppen, and D.G. Hummer: Ap.J. **331**, 815 (1988)

I. Hubeny, D.G. Hummer, and T. Lanz: Astron. Astrophys. **282**, 151 (1994)

A. Nayfonov, W. Däppen, D.G. Hummer, and D. Mihalas: Ap.J. **526**, 451 (1999)



Occupation probabilities w

- charged particle (plasma microfield $P(F)$)
perturbations of atomic structure

$$w_{mf} = \int_0^{F_c} P(F) dF \quad ; F_c - \text{critical microfield}$$

- finite-size effects

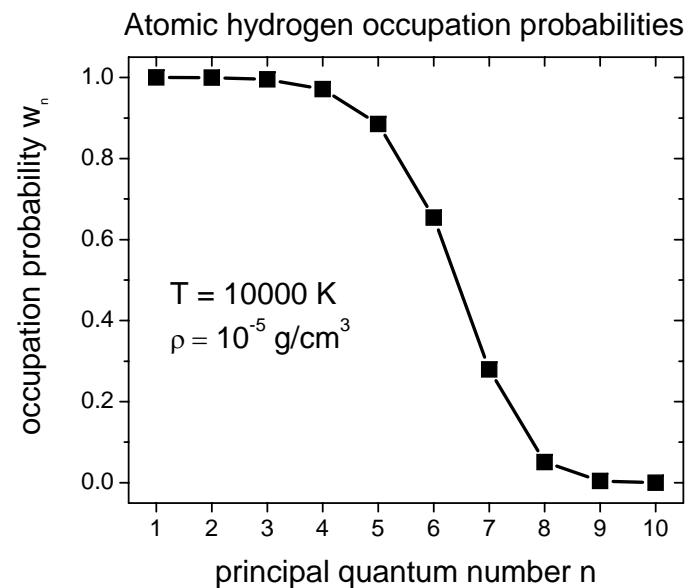
$$w_{hs} \propto \text{excluded volume}$$

- convergent partition function

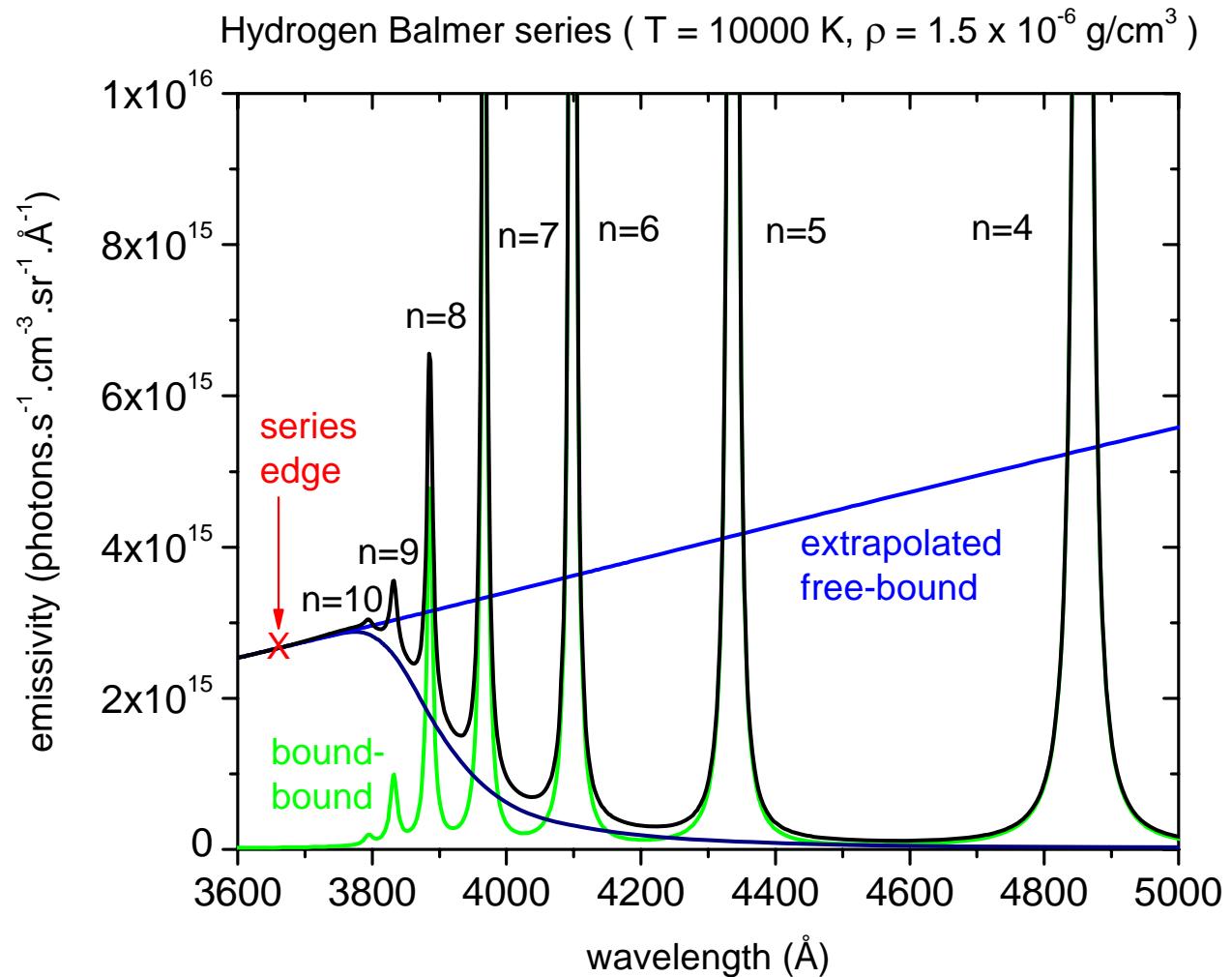
$$\tilde{Z} = \sum_j w_j g_j \exp(-E_j/kT)$$

- LTE level populations N_j

$$N_j/N_T = w_j g_j \exp(-E_j/kT)/\tilde{Z}$$



Spectral line series edge broadening



W. Däppen, L. Anderson, and D. Mihalas: Ap.J. **319**, 195 (1987)

I. Hubeny, D.G. Hummer, and T. Lanz: Astron. Astrophys. **282**, 151 (1994)



Helmholtz free energy contributions

$$F = -kT \ln Z$$

- chemical picture \leftrightarrow partition function factorization

$$F = F_1 + F_2 + F_3 + F_4 + F_5$$

- F_1 - ions, translational (classical)
- F_2 - ions, internal (partition functions \tilde{Z})
- F_3 - electrons, with degeneracy effects
- F_4 - Coulomb interaction plasma term
- F_5 - finite atom size effects (pressure ionization)

Free energy contributions, cont.

- F_1 - ions, translational (classical ideal gas)

$$F_1 = kT \sum_{s \neq e} N_s \left[\ln \left(\frac{N_s \Lambda_s^3}{V g_s} \right) - 1 \right] \quad \Lambda_s = \sqrt{\frac{2\pi\hbar^2}{m_s kT}}$$

- F_2 - ions, internal (excited states)

$$F_2 = \sum_{s \neq e} N_s \left(E_{s1} - kT \ln \tilde{Z}_s \right) \quad \tilde{Z}_s = \sum_j w_{sj} g_{sj} \exp \left(- \frac{E_{sj} - E_{s1}}{kT} \right)$$

A.Y. Potekhin, G. Chabrier, and D. Gilles, Phys. Rev. E **65**, 036412 (2002)

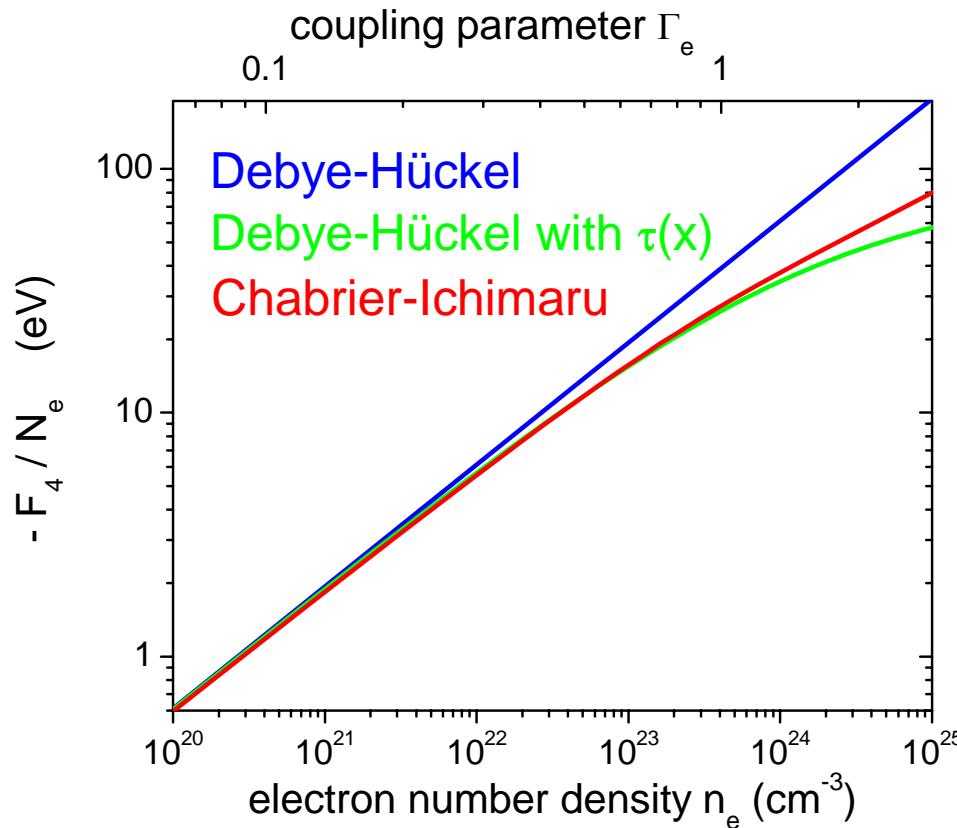
- F_3 - electrons: ideal, partially degenerate Fermi gas

$$F_3 = kT N_e \left(\eta - I_{3/2}(\eta) / I_{1/2}(\eta) \right) \quad I_{1/2}(\eta) = \frac{N_e \Lambda_e^3}{2V}$$



Free energy contributions, cont.

- F_4 - Coulomb interaction plasma term

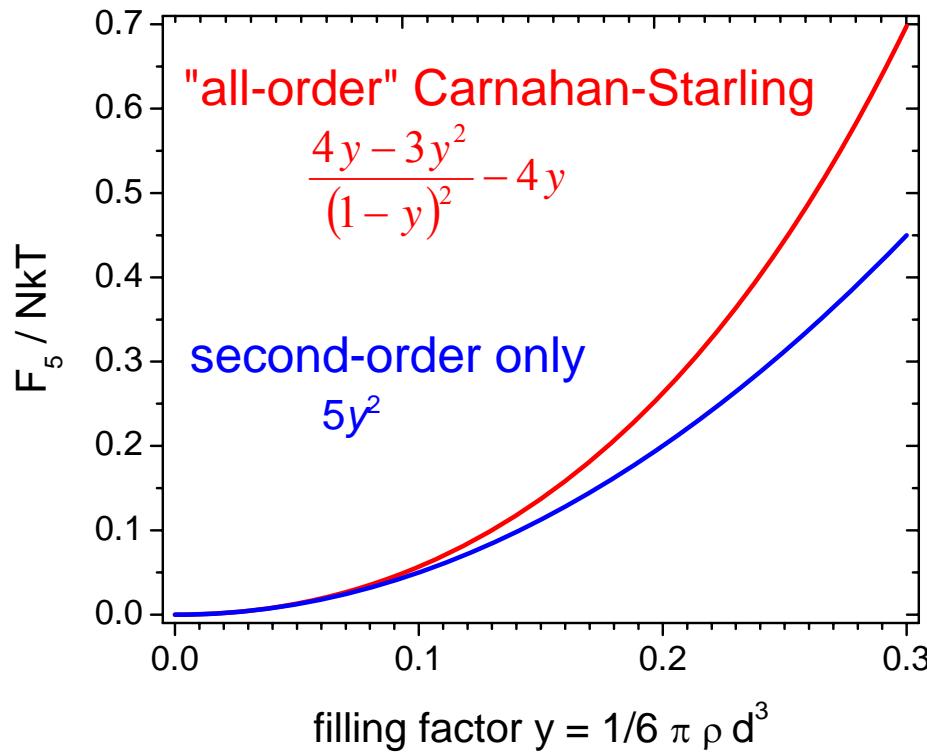


example:
fully ionized hydrogen
 $T = 200,000 \text{ K}$

G. Chabrier and A.Y. Potekhin, Phys. Rev. E **58** (4), 4941 (1998); **62** (6) 8554 (2000)
S. Ichimaru, H. Iyetomi, and S. Tanaka, Phys. Rep. **149** (2&3), 91 (1987)

Free energy contributions, cont.

- F_5 - finite atom size effects (pressure ionization), mixture of hard spheres



example:
one-component
hard-sphere system:
 d – hard-sphere diameter
 ρ – particle number density

N.F. Carnahan and K.E. Starling, J. Chem. Phys. **51** (2), 635 (1969)

Free energy contributions, cont.

- simple hard-sphere description becomes inadequate at high densities
- liquid perturbation theories: known reference system plus corrections (Barker-Henderson, and Weeks-Chandler-Andersen, ...)

$$F_5 = F_5^{ref} + \frac{N^2}{2V} \int d\vec{r} g_{ref}(r) u_{attract}(r) + \dots$$

- soft-sphere model = hard-sphere reference system with density- (and temperature-) dependent radii
- effective radii values calibrated by comparisons with *ab initio* calculations such as QMD, PIMC

Minimizing F : initialization

- solve a system of Saha-type equations derived from stoichiometric constraints:

$dF = 0$ for process $A^{m+} \leftrightarrow A^{(m+1)+} + e^-$ yields,

$$\frac{n_{m+1}}{n_m} = \frac{\tilde{Z}_{m+1}}{\tilde{Z}_m} \exp\left[-\left(\chi_{m,m+1} - \phi_m + \mu_e^{(0)}\right)/kT\right]$$

- analogous equations for molecular dissociation
- closure provided by:

- total mass conservation

$$N_{total} = \sum_{m \neq e} a_m N_m$$

- charge neutrality condition

$$N_e = \sum_{m \neq e} z_m N_m$$



Helmholtz free energy contributions in the Saha-based initialization model

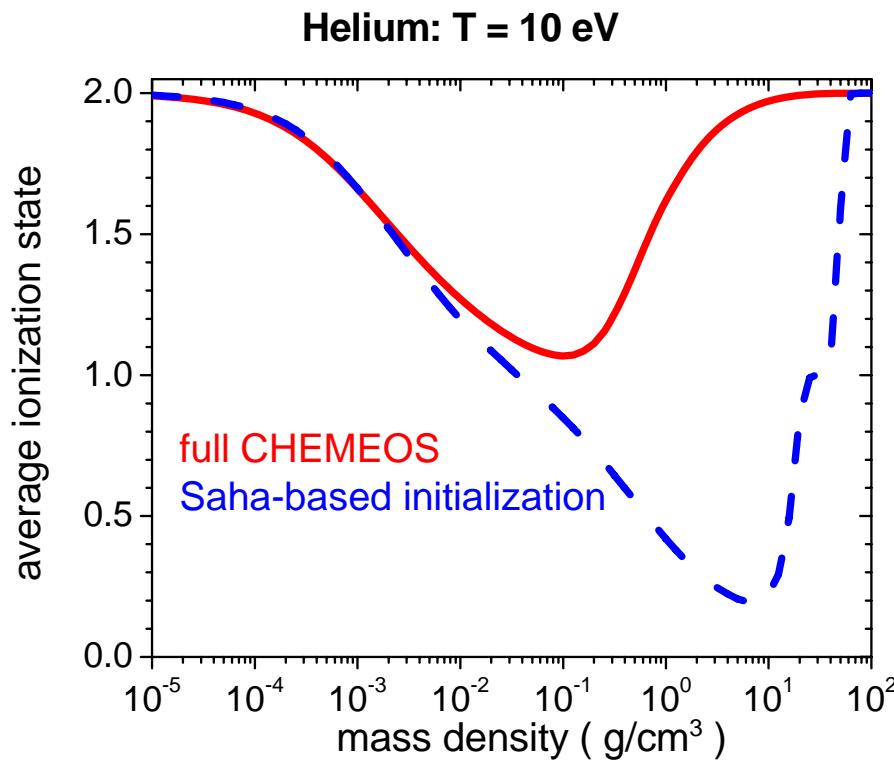
$$F = -kT \ln Z$$

$$F = F_1 + F_2 + F_3 + F_4 + F_5$$

- F_1 - ions, translational (classical): full account
- F_2 - ions, internal: ground-states only (see also F_5)
- F_3 - electrons, with degeneracy effects: full account
- F_4 - Coulomb interaction term:
Stewart-Pyatt continuum-lowering formula
- F_5 - finite atom size effects (pressure ionization):
density-dependent occupation probabilities of
ground states in F_2

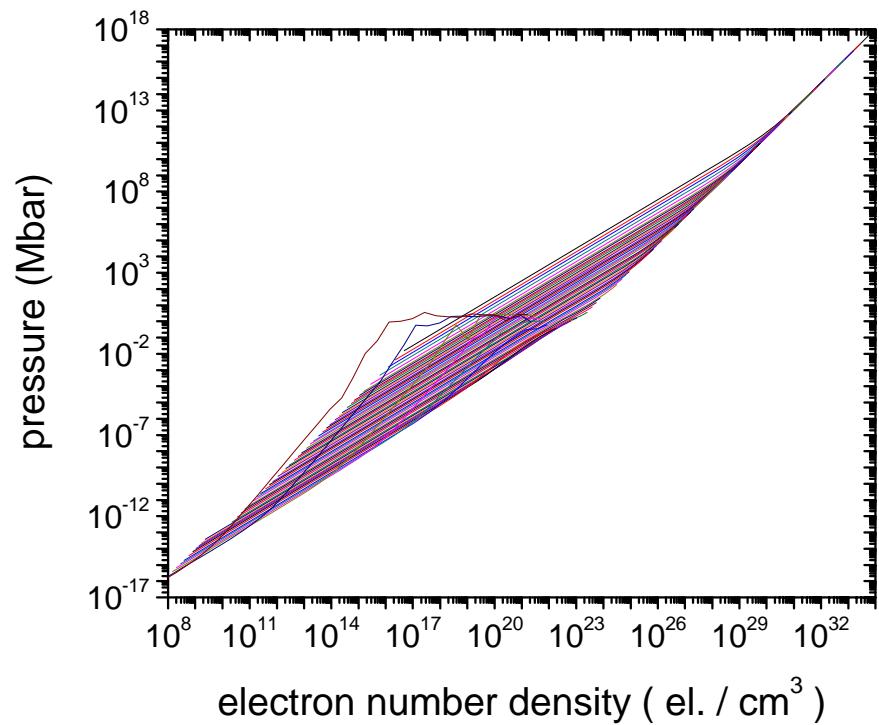
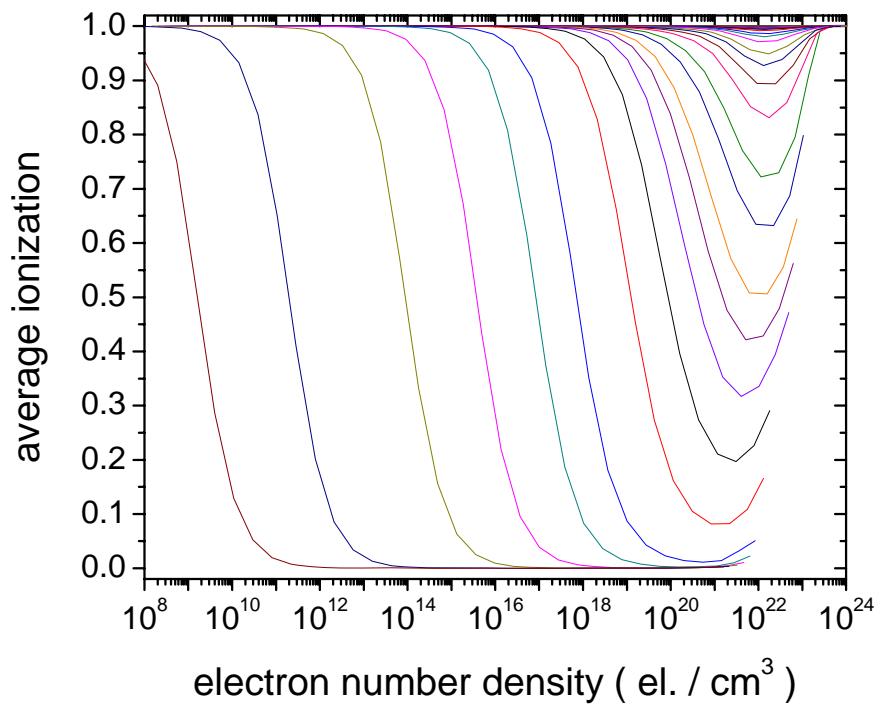
Minimizing F : continued...

- Powell method (no use of gradients) with the "Saha-based solution" providing the initial guess
- truncated-Newton algorithm (Stephen Nash); use of gradients should speed up code (future work)



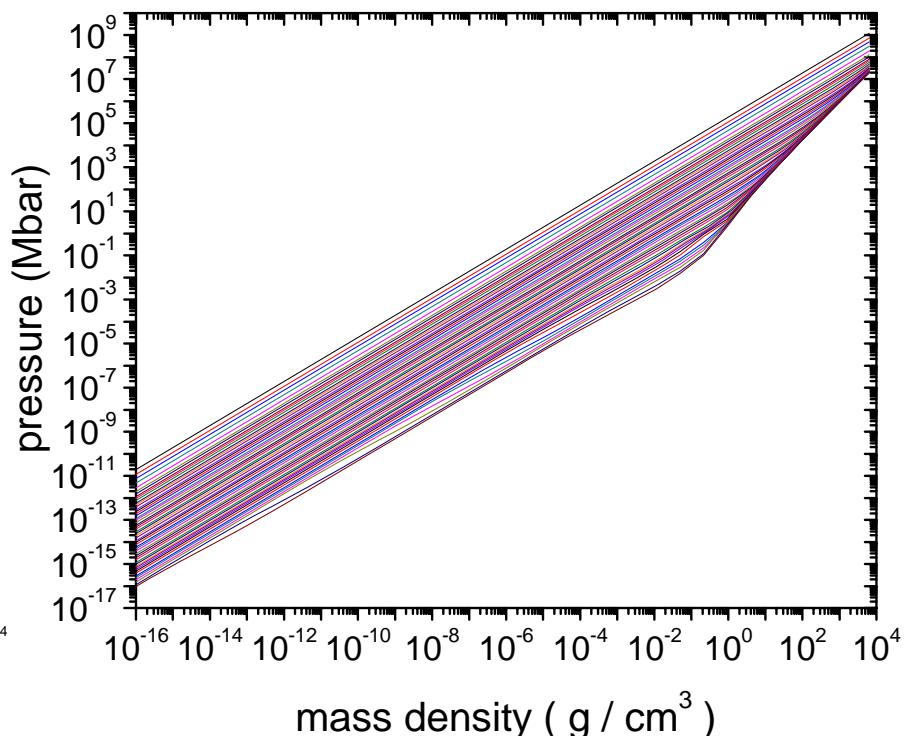
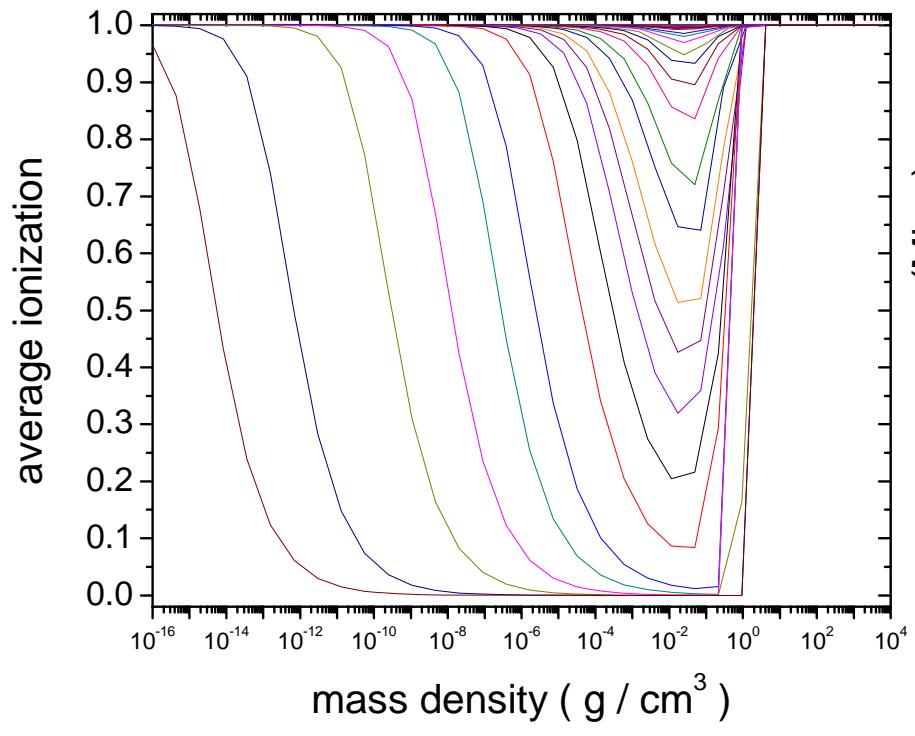
Hydrogen table

electron number density on input



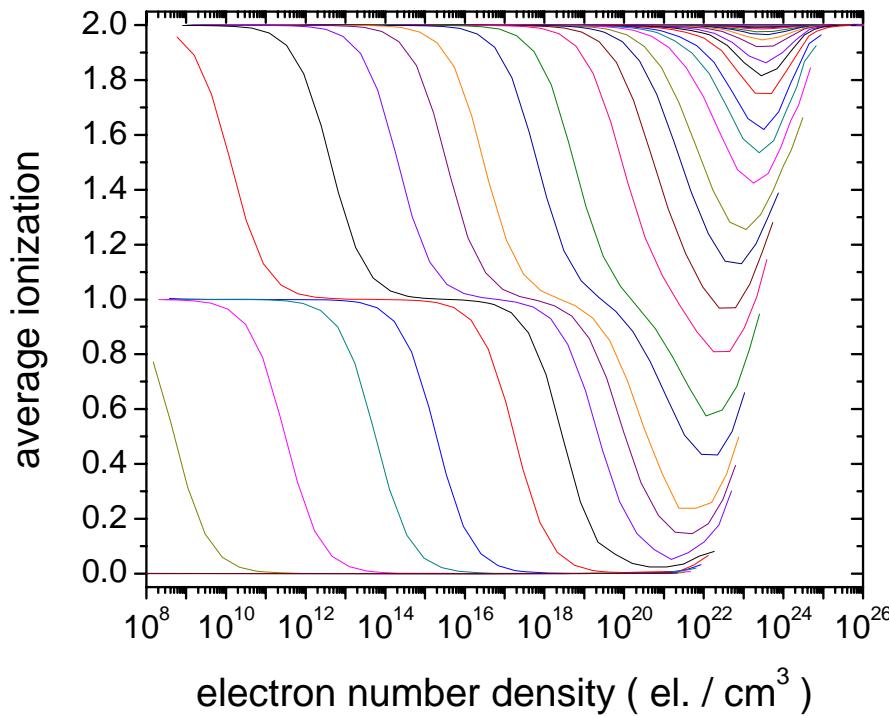
Hydrogen table

mass density on input

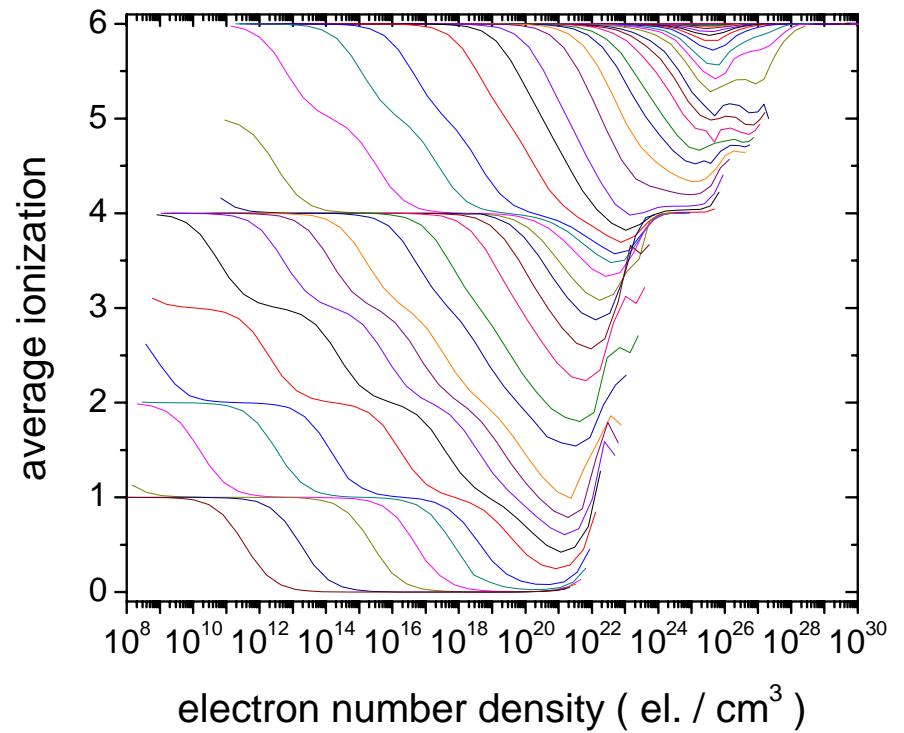


Helium and Carbon tables

electron number density on input



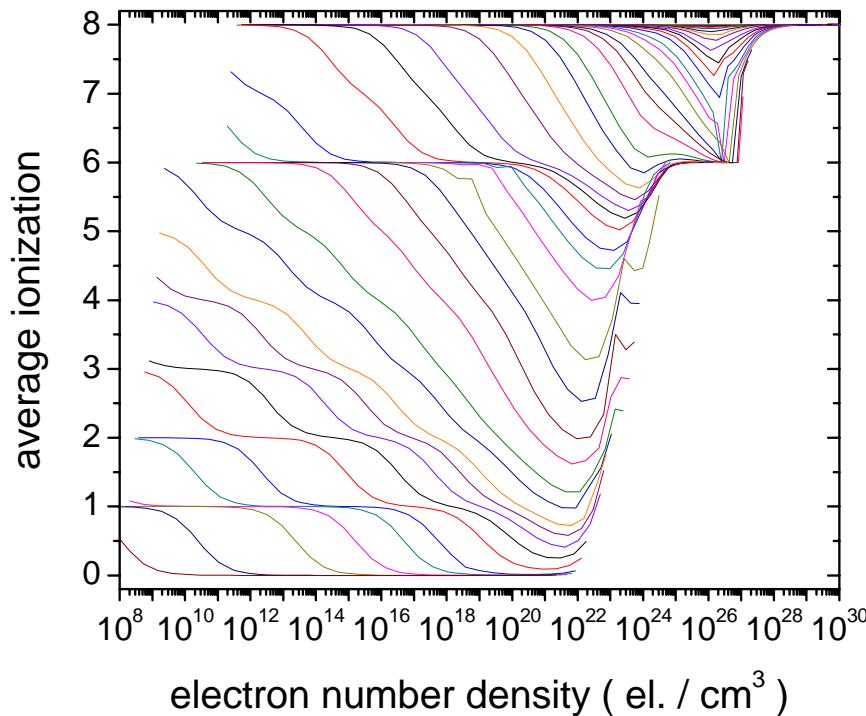
Helium



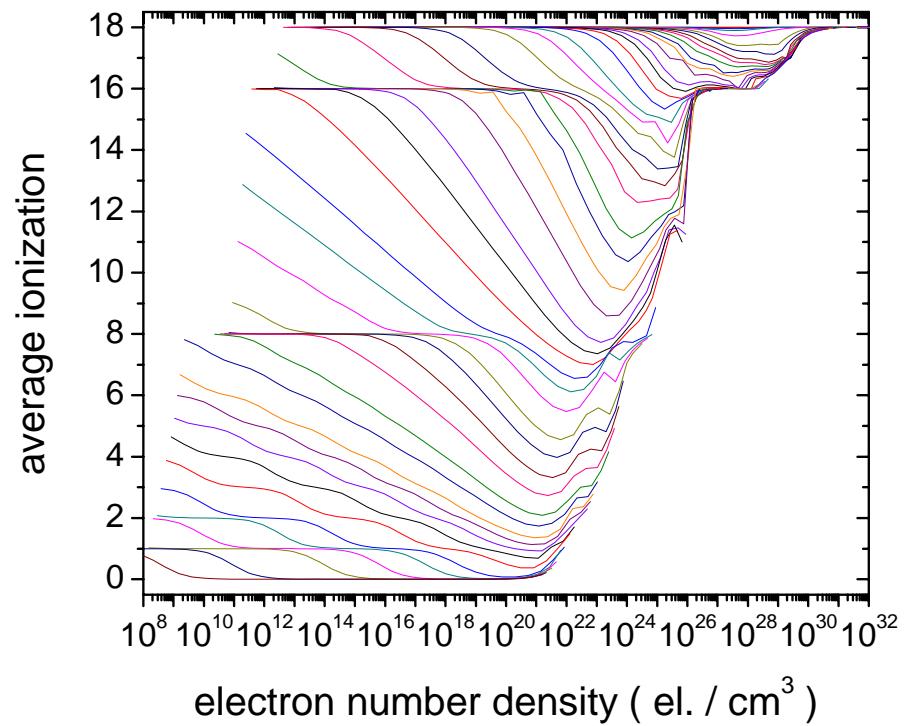
Carbon

Oxygen and Argon tables

electron number density on input

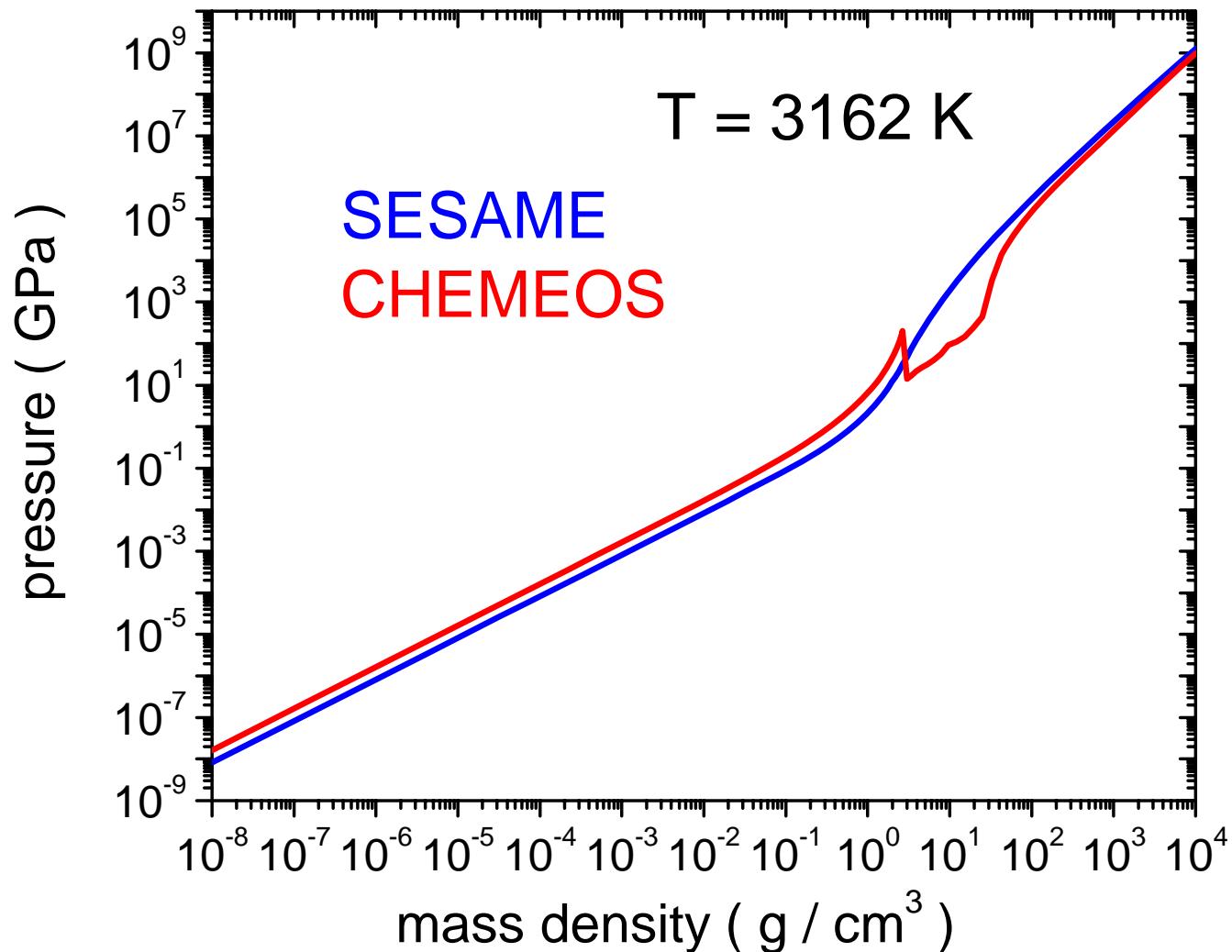


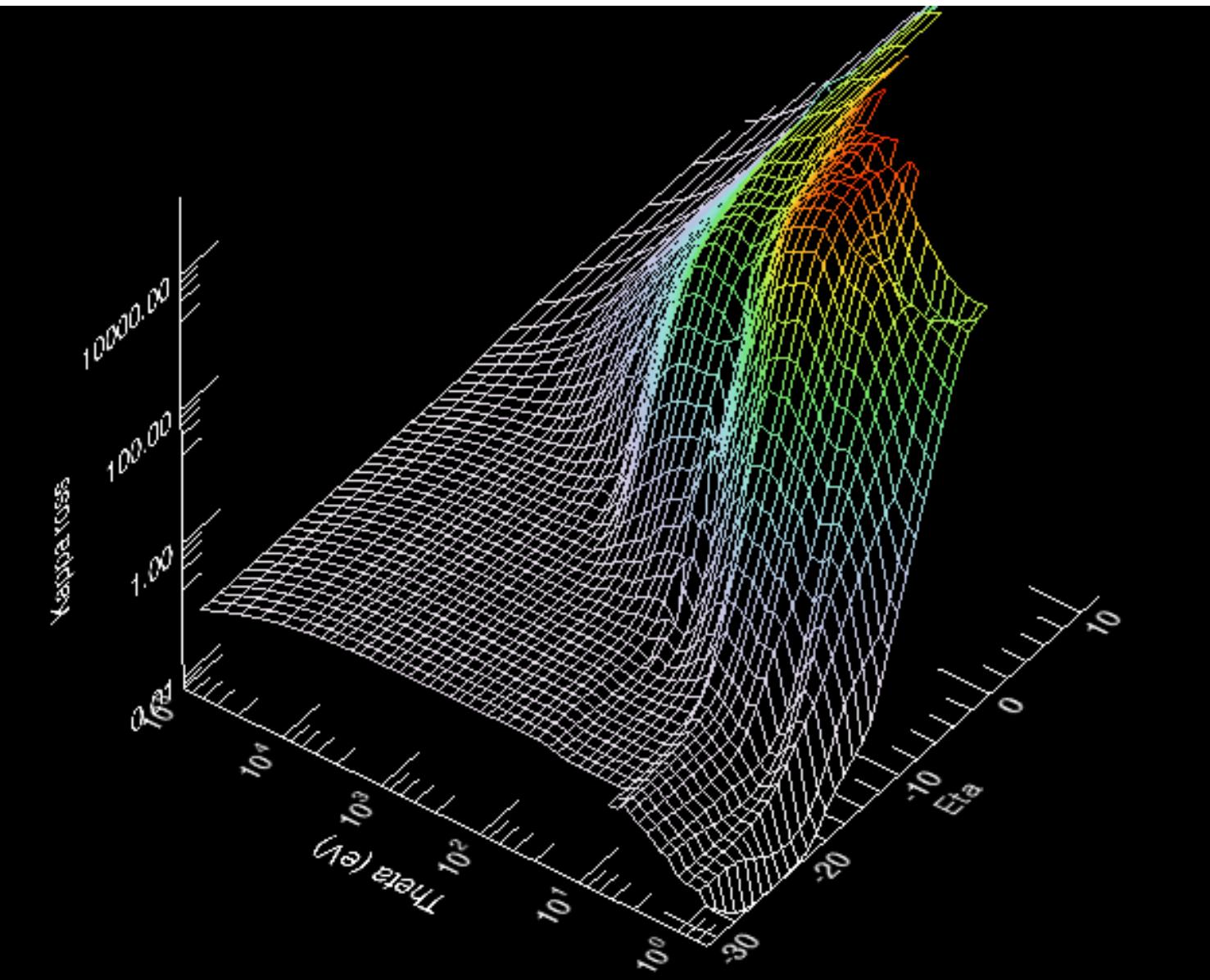
Oxygen



Argon

OXYGEN





Occupation probabilities

H-like CARBON: $T = 10^6$ K, $\rho = 0.01$ g / cm³

n	CHEMEOSt	Holtsmark*	OP*	APEX*	OPAL*
1	1.00	1.00	1.00	1.00	1.00
2	1.00	9.97E-1	9.91E-1	9.98E-1	9.96E-1
3	9.87E-1	9.50E-1	9.06E-1	9.76E-1	9.95E-1
4	7.08E-1	4.90E-1	4.95E-1	7.20E-1	9.95E-1
5	1.25E-1	5.25E-2	3.62E-2	1.76E-1	9.14E-1
6	1.14E-2	4.63E-3	6.33E-6	2.21E-2	5.27E-1
7	1.04E-3	5.19E-3	2.96E-16	2.46E-3	1.62E-1
8	9.58E-5	7.79E-5	4.76E-41	3.66E-4	2.37E-2
9	7.63E-6	3.19E-6	1.06E-94	6.75E-5	2.23E-3

† A.Y. Potekhin, G. Chabrier, and D. Gilles, Physical Review E **65**, 036412 (2002)

* C.A. Iglesias and F.J. Rogers, Astrophysical Journal **443**, 460-463 (1995)



Summary and future work

- new low-Z opacity and EOS code ATOMIC
- chemical picture
- free-energy minimization method
- occupation-probability formalism
- analytic equations of state
- self-consistent opacity and EOS data
- application to non-LTE
- better microfields (unscreened → screened)
- application to heavier elements